

	Hits	Search Text
1	2	("6262085").PN.
2	2	("6150380").PN.
3	2	("6268385").PN.
4	2	("20020004512").PN.
5	2461	(436/171,164,106).CCLS.
6	1	((436/171,164,106).CCLS.) and omeprazole\$2
7	1957	omeprazole\$2
8	387	omeprazole\$2 and spectr\$4
9	2	("6262085").PN.
10	0	Whittle.inv. and Raman and omeprazol
11	768	Whittle.inv.
12	0	S11 and omeprazol
13	40	S11 and Raman
14	3	"200113919"
15	2	("6667323").PN.
16	2	("6780880").PN.
17	44	isomer\$2 with Raman
18	41	S17 and (calibrat\$2 or standard\$2 or reference\$2)
19	3	S17 and calibrat\$2
20	710	isomer\$2 and Raman
21	115	S20 and calibrat\$2
22	0	S21 and (isomer\$2 near2 ratio\$2)
23	36	S20 and (isomer\$2 near2 ratio\$2)

10651225

FILE 'CAPLUS' ENTERED AT 15:53:29 ON 21 JUN 2005

L1 1549 ISOMER? (S) RAMAN

L2 5 L1 AND CALIBRAT?

L3 18 L1 AND (ISOMER? (3A) RATIO?)

L2 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:1012039 CAPLUS

DOCUMENT NUMBER: 141:419933

TITLE: Spectroscopic determination of the isomeric composition of aromatic isocyanate mixtures

INVENTOR(S): Mahrenholtz, Jochen; Wimschneider, Andrea; Pirkel, Hans-Georg; Mueller, Heinz-Herbert; Dresely, Stefan; Bolton, Jeffrey; Schiffhauer, Martin; Wolf, Udo; Schweer, Johannes; Gerlach, Martin

PATENT ASSIGNEE(S): Bayer Materials Science AG, Germany

SOURCE: Eur. Pat. Appl., 18 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

PATENT NO. KIND DATE APPLICATION NO. DATE

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EP 1480033 A1 20041124 EP 2004-10763 20040506  
DE 10322439 A1 20041209 DE 2003-10322439 20030519  
CA 2467281 AA 20041119 CA 2004-2467281 20040514  
US 2005003553 A1 20050106 US 2004-845727 20040514  
JP 2004347598 A2 20041209 JP 2004-147303 20040518  
BR 2004001771 A 20050125 BR 2004-1771 20040518

PRIORITY APPLN. INFO.: DE 2003-10322439 A 20030519

AB The isomeric composition of an isocyanate mixture is determined by NIR, Raman, or mid-IR spectroscopy and subjecting the spectral data to a chemometric calibration model using the partial least square method. The isocyanates are aromatic isocyanates, such as naphthylene diisocyanate, xylylene diisocyanate, methylene-diphenyl diisocyanate, or toluene diisocyanate (TDI). The results are used for the automatic control of the isocyanate production process. REFERENCE COUNT: 6

L2 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:572237 CAPLUS

DOCUMENT NUMBER: 137:262043

TITLE: Evaluation of Raman Spectroscopy for Determining cis and trans Isomers in Partially Hydrogenated Soybean Oil

AUTHOR(S): Johnson, G. L.; Machado, R. M.; Freidl, K. G.; Achenbach, M. L.; Clark, P. J.; Reidy, S. K.

CORPORATE SOURCE: Air Products and Chemicals Inc., Allentown, PA, 18195-1501, USA

SOURCE: Organic Process Research & Development (2002), 6(5), 637-644

CODEN: OPRDFK; ISSN: 1083-6160  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The determination of trans isomer content in partially hydrogenated vegetable oils is important in the characterization of fats and oils in the food industry. Current methods for characterization include gas chromatog. and IR spectroscopy of samples captured off-line. The determination of trans isomer content during the hydrogenation process has the potential to improve process productivity and quality control to meet the stringent requirements of oil producers. Raman spectroscopy was evaluated in comparison to IR spectroscopy as a method for quant. determining the cis and trans isomer content in partially hydrogenated vegetable oils. Both IR and Raman principal component regression (PCR) calibrations accurately modeled the GC values (AOCS Official Method Ce 1f-96) for cis and trans content. In addition, the cis and trans isomer content of canola oil could be determined after the results from the IR and Raman calibration methods for soybean oil were corrected for slope and offset. Raman spectroscopy possesses unique advantages and shows promise as a method for rapid in situ anal.

REFERENCE COUNT: 20

L2 ANSWER 3 OF 5 CAPLUS. COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:517052 CAPLUS

DOCUMENT NUMBER: 137:201065

TITLE: Global Quantitation of Solvent Effects on the Isomerization Thermodynamics of 1,2-Dichloroethane and trans-1,2-Dichlorocyclohexane

AUTHOR(S): McClain, Brian L.; Ben-Amotz, Dor

CORPORATE SOURCE: Department of Chemistry, Purdue University, West Lafayette, IN, 47907-1393, USA

SOURCE: Journal of Physical Chemistry B (2002), 106(32), 7882-7888

CODEN: JPCBFK; ISSN: 1089-5647

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The conformational equilibrium of the trans-gauche isomerization of 1,2-dichloroethane (DCE) and the axial, axial-equatorial, equatorial isomerization of trans-1,2-dichlorocyclohexane (T12D), both dissolved in di-Et ether, are studied using Raman spectroscopy. The C-Cl stretch band areas of the two conformers are measured as a function of temperature and pressure. The resulting area ratios, calibrated against NMR measurements, are used to globally quantitate the complete set of isomerization thermodyn. functions in solution, as well as the corresponding solvent excess contributions (by comparison with vapor-phase results). The effects of pressure on the two isomerization processes are found to be opposite in sign, as the polar isomer (gauche) of DCE is favored at high pressure and low temperature, while the more polar (equatorial, equatorial) form of T12D is driven in the opposite direction. The excess enthalpy (and energy) of reaction is neg. for both reactions, while the reaction volume is neg. for the DCE and pos. for T12D. The results reveal the different impact of attractive (cohesive)

and repulsive (cavity formation) perturbations on various thermodyn. functions.

REFERENCE COUNT: 61

L2 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:807644 CAPLUS

DOCUMENT NUMBER: 123:358141

TITLE: "Determination of enantiomeric excess using Raman optical activity"

AUTHOR(S): *Hecht, Lutz; Phillips, Anthony; Barron, Laurence D.*

CORPORATE SOURCE: Chem. Dep., Univ. Glasgow, G12 8QQ, UK

SOURCE: **Journal of Raman Spectroscopy (1995), 26(8 & 9), 727-32**

CODEN: JRSPAF; ISSN: 0377-0486

PUBLISHER: Wiley

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A simple method for the determination of enantiomeric excess is described. It is based on depolarized Raman optical activity (ROA) measurements in right-angle scattering employing the incident circular polarization (ICP) modulation approach. The accuracy of this method was assessed using <SYM97>-pinene as a chiral test compound. The four <SYM97>-pinene ICP ROA signals associated with the Raman bands observed at .apprx.772, 787, 887, and 929 cm<sup>-1</sup> were selected to establish a linear relationship between ROA signal strength and enantiomeric composition for a set of calibration mixts. containing both <SYM97>-pinene enantiomers. Using this relation a (+)-<SYM97>-pinene sample content of 16.3% was determined for a blind mixture containing 83.6% (1S)-(-)-<SYM97>-pinene and 16.4% (1R)-(+)-<SYM97>-pinene. Similarly, using addnl. spectral subtraction procedures, a (+)-<SYM97>-pinene sample content of 1.5% was estimated for a test mixture consisting of 50.1% (1S)-(-)-<SYM97>-pinene and 49.9% (1S)-(-)-trans- pinane.

L2 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:575216 CAPLUS

DOCUMENT NUMBER: 87:175216

TITLE: "Determination of the sample temperature from the intensity ratio of Stokes and anti-Stokes lines; photometric calibration of Raman spectrometers. Determination of <SYM68>H and <SYM68>S of conformational isomers"

AUTHOR(S): *Spiekermann, M.; Schrader, B.; D'Orazio, M.*

CORPORATE SOURCE: Inst. Spektrochem., Univ. Dortmund, Dortmund, Fed. Rep. Ger.

SOURCE: **Proc. Int. Conf. Raman Spectrosc., 5th (1976), 346-7.** Editor(s): Schmid, Eduard D.; Brandmueller, J.; Kiefer, W. Hans Ferdinand Schulz Verlag: Freiburg/Br., Ger.

CODEN: 36RDA9

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The illuminated sample temperature was determined from the Raman intensity ratio of Stokes and anti-Stokes lines by using the equation given by G. Placzek (1934). The spectral response of the spectrometer was calibrated by the method of M. D'Orazio and

B. Schrader (1974). The determination of <SYM68>H and <SYM68>S of conformational isomers from Raman intensities is analogous to the procedure developed for IR spectra by H. Braun (1974); instead of the extinction  $E_k$ , the Raman intensity  $I_k$  is evaluated. The evaluation of the integral intensities for the Raman bands at 551 and 659  $\text{cm}^{-1}$  for the gauche and trans isomer of 1,2-dibromoethane gave the following values: <SYM68>H =  $658 \pm 35$  cal/mol; <SYM68>S =  $1.92 \pm 0.2$  cal/mol.

L3 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:152490 CAPLUS

DOCUMENT NUMBER: 134:198192

TITLE: *FT-Raman spectroscopic measurement of omeprazole isomer ratio in a composition*

INVENTOR(S): Whittle, Robert R.; Sancilio, Frederick D.; Stowell, Grayson Walker

PATENT ASSIGNEE(S): Applied Analytical Industries, Inc., USA

SOURCE: PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2001013919 A1 20010301 WO 2000-US23368 20000823

CA 2382838 AA 20010301 CA 2000-2382838 20000823

AU 2000069377 A5 20010319 AU 2000-69377 20000823

EP 1206263 A1 20020522 EP 2000-957808 20000823

JP 2003507721 T2 20030225 JP 2001-518056 20000823

US 6780880 B1 20040824 US 2000-649447 20000825

ZA 2002001519 A 20030522 ZA 2002-1519 20020222

ZA 2002001521 A 20030522 ZA 2002-1521 20020222

PRIORITY APPLN. INFO.: US 1999-150878P P 19990826

WO 2000-US23368 W 20000823

AB *Fourier-transform Raman spectroscopy (FT-Raman) detcs. the isomer ratio of chemical compns., especially the ratio of 5(6)-methoxy isomers of omeprazole. An omeprazole active pharmaceutical ingredient (API) composition fixed with a ratio of 5(6)-methoxy isomers is also disclosed. REFERENCE COUNT: 6*

L3 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:624192 CAPLUS

DOCUMENT NUMBER: 133:277799

TITLE: "Picosecond Time-Resolved Resonance Raman Study of the Photoisomerization of Retinal"

AUTHOR(S): Shimojima, Atsuhiko; Tahara, Tahei

CORPORATE SOURCE: Institute for Molecular Science, Myodaiji, Okazaki, 444-8585, Japan

SOURCE: **Journal of Physical Chemistry B (2000), 104(39), 9288-9300**

CODEN: JPCBFK; ISSN: 1089-5647

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

**AB** Picosecond time-resolved Raman spectroscopy was applied to the study of the photoisomerization dynamics of all-trans, 9-cis and 13-cis retinal in nonpolar solvents. It was found that picosecond time-resolved spontaneous Raman spectra are obtainable from retinal in solution despite a high fluorescence background when the probe wavelength is in rigorous resonance with the T-T absorption. In the case of photoexcitation of all-trans retinal, the transient Raman bands ascribed to the all-trans T1 state appeared with the intersystem crossing time of .apprx.30 ps. No Raman signal attributable to the product was recognized within the signal-to-noise ratio, reflecting the low isomerization quantum yield of all-trans retinal. The frequency shifts of the all-trans T1 bands were observed in the early picosecond time region (<SYM116> .apprx. 16 ps), which manifests the vibrational cooling process in the excited state. In the case of photoexcitation of 9-cis retinal, the all-trans T1 state slowly appeared with a time constant of .apprx.1 ns ( $1000 \pm 150$  ps), which corresponds to the 9-cis <SYM174> all-trans structural change occurring in the T1 state. In addition, Raman signals due to the 9-cis T1 state (e.g., 1400 cm<sup>-1</sup>) were recognized in the early delay time and they disappeared in accordance with the appearance of the all-trans T1 state. The data obtained clearly showed that the 9-cis <SYM174> all-trans photoisomerization predominantly takes place in the T1 state with thermal activation to cross the potential barrier from the 9-cis configuration to the all-trans. In contrast, with photoexcitation of 13-cis retinal, the transient Raman signals attributable to the mixture of the all-trans T1 state and the 13-cis T1 state appeared in a few tens of picoseconds, and no spectral change was observed after 100 ps up to a few nanoseconds. The quant. anal. indicated that the all-trans T1 state and the 13-cis T1 state appeared with different time consts. It suggests that the 13-cis <SYM174> all-trans isomerization takes place in the excited singlet state before the intersystem crossing and that the resultant all-trans S1 and 13-cis S1 states are relaxed to the corresponding T1 states sep. with time consts. inherent to each isomer. The singlet isomerization quantum yield was estimated approx. at .apprx.0.2 from the obtained picosecond Raman data. These results indicated that the singlet mechanism is a major pathway (or one of major pathways) in photoisomerization of 13-cis retinal. The present time-resolved Raman study showed that the cis <SYM174> trans photoisomerization mechanism and dynamics of retinal significantly depend on the position of the double bond to rotate.

REFERENCE COUNT: 55

L3 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:544600 CAPLUS

DOCUMENT NUMBER: 129:230359

TITLE: "Mechanism and potential energy surface for photoisomerization of stilbene in zeolite nanospace"

AUTHOR(S): *Kuriyama, Yasunao; Takeya, Haruhiko; Oishi, Shigero; Kojima, Masanobu*

CORPORATE SOURCE: Department of Chemistry, School of Science, Kitasato University, Kanagawa, 228-8555, Japan

SOURCE: **Chemistry Letters (1998), (8), 843-844**

CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The photoisomerization of cis- and trans-stilbenes adsorbed in zeolite supercage was studied by means of Raman spectroscopy for in situ anal. of the isomer ratio in the photostationary state. It was found that the isomerization proceeds mainly through the singlet excited states for NaY and triplet excited states for KY, and also a new potential energy surface for the photoisomerization was proposed. REFERENCE COUNT: 20

L3 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:526724 CAPLUS

TITLE: Photoisomerization mechanism of stilbene adsorbed in Y zeolite

AUTHOR(S): Kuriyama, Y.; Kojima, M.; Takeya, H.; Oishi, S.

CORPORATE SOURCE: Department Chemistry, Kitasato University, Kanagawa, 228-8555, Japan

SOURCE: Book of Abstracts, 216th ACS National Meeting, Boston, August 23-27 (1998), PHYS-285. American Chemical Society: Washington, D. C.

CODEN: 66KYA2

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB We have investigated the photoisomerization of cis- and trans-stilbenes in the supercages of zeolites NaY and KY without solvent. We succeeded to determine c-St/t-St isomer ratio at photostationary state (PSS) by means of Raman spectroscopy. This method is very useful for in situ anal. We obtained PSS and found trans-isomer is predominate in the zeolite cage. To explain these phenomena, we propose that the potential energy surface for stilbene isomerization in zeolite cage will be different from that of solution

L3 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:801059 CAPLUS

DOCUMENT NUMBER: 123:223108

TITLE: Resonance Raman evidence for 15-cis to all-trans photoisomerization of spirilloxanthin bound to a reduced form of the reaction center of Rhodospirillum rubrum S1

AUTHOR(S): Kuki, Michitaka; Naruse, Mitsuru; Kakuno, Tomisaburo; Koyama, Yasushi

CORPORATE SOURCE: Faculty Science, Kwansei Gakuin University, Nishinomiya, 662, Japan

SOURCE: Photochemistry and Photobiology (1995), 62(3), 502-8

CODEN: PHCBAP; ISSN: 0031-8655

PUBLISHER: American Society for Photobiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reaction center (RC) of R. rubrum S1, which was prepared by ultrafiltration, showed one peak in mol.-sieve HPLC, but it showed two peaks in diethylaminoethyl

(DEAE) ion-exchange HPLC; they were named a sRC-<SYM97> and RC-<SYM98> in the order of elution, nonequilibrated isoelec. electrophoresis, together with DEAE ion-exchange HPLC, showed that RC-<SYM98> is electronically more neg. than RC-<SYM97>. Oxidation of RC-<SYM98> by addition of ferricyanide caused its transformation into RC-<SYM97>, while reduction of RC-<SYM97> by adding ascorbate and subsequent illumination caused its transformation into RC-<SYM98>. Resonance Raman spectroscopy of the RC at liquid nitrogen temperature detected the all-trans and the 15-cis isomers in a ratio of 1:1, but HPLC analyses of the carotenoid extracted from the RC before and after the Raman measurements detected the pair of isomers in a ratio of 1:6. Thus, the 15-cis to all-trans isomerization takes place during irradiation at liquid nitrogen temperature, while the reverse isomerization takes place in the dark. The isolated RC-<SYM97> and dRC-<SYM98> exhibited the bleaching of the 868 nm band, and contained the H, M and L subunits and 1.2-1.4 mols. of ubiquinone-10 per RC. Each RC slowly equilibrated in the dark toward a mixture of RC-<SYM97> and RC-<SYM98>. Generation of the all-trans isomer in the light was found not in RC-<SYM97> but in RC-<SYM98>.

L3 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:355356 CAPLUS

DOCUMENT NUMBER: 122:181293

TITLE: "Equilibrium composition of retinal isomers in dark-adapted bacteriorhodopsin and effect of high pressure probed by near-infrared Raman spectrometry"

AUTHOR(S): *Schulte, A.; Bradley, L., II; Williams, C.*

CORPORATE SOURCE: Cent. Res. Educ. Opt. Lasers, Univ. Cent. Florida, Orlando, FL, 32816-2385, USA

SOURCE: **Applied Spectroscopy (1995), 49(1), 80-3**

CODEN: APSPA4; ISSN: 0003-7028

PUBLISHER: Society for Applied Spectroscopy

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The combination of near-IR Raman spectroscopy and variations in external parameters offers new opportunities for site-specific studies of proteins. Using excitation at 840 nm, the authors measured the near-IR Raman spectrum of dark-adapted bacteriorhodopsin at ambient and high pressure. The C:C ethylenic stretching region showed 2 resolved bands at 1526 and 1534 cm<sup>-1</sup>, corresponding to the all-trans and 13-cis isomers. From deconvolution of these bands, an isomeric ratio between 13-cis- and all-trans-retinal of 1 at ambient pressure was found. The Raman spectrum gave direct spectroscopic evidence that the 13-cis component was favored at high pressure, implying that it has a smaller volume. The pressure dependence of the isomeric ratio yielded a molar volume of -6.6 mL/mol, which suggests ionization of 1 or 2 residues or the formation of 3 H-bonds.

L3 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:207714 CAPLUS

DOCUMENT NUMBER: 114:207714

TITLE: "Ultraviolet resonance Raman study of proline isomerization"



AUTHOR(S): Harhay, Gregory P.; Hudson, Bruce S.  
CORPORATE SOURCE: Inst. Mol. Biol., Univ. Oregon, Eugene, OR, 97403, USA  
SOURCE: Journal of Physical Chemistry (1991), 95(9), 3511-13  
CODEN: JPCHAX; ISSN: 0022-3654  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The UV resonance Raman spectra of aqueous solns. of proline dipeptides obtained with 200- and 218-nm excitation at pH 1.5 and 6.5 are reported. The cis/trans isomer ratio for these dipeptides is known to depend on pH. The amide II' like mode of the X-Pro peptide (imide) linkage at 1487 cm<sup>-1</sup>, involving predominantly the motions of the peptide carbon and nitrogen, is the most strongly enhanced band in the 200-250 nm region. This band does not shift appreciably with the change in isomer ratio associated with the change in pH. The same behavior is observed with the 1467-cm<sup>-1</sup> band of aqueous polyproline, which has undergone a salt-induced isomerization. Contrary to earlier evidence, the position of the amide II' like band is not diagnostic for the isomeric state of the imide bond.

L3 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1967:468950 CAPLUS  
DOCUMENT NUMBER: 67:68950  
TITLE: Infrared spectra and rotamers of a few ethylchlorosilanes  
AUTHOR(S): Pentin, Yu. A.; Rudakova, S. E.  
CORPORATE SOURCE: Gos. Univ., Moscow, USSR  
SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1967), 51(3), 285-94  
CODEN: ACASA2; ISSN: 0001-5407  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian

AB The ir, in the solid, liquid, and vapor state, and the Raman spectra, in the solid and liquid state, in the 400-3000cm.<sup>-1</sup> region were obtained as a means of studying the rotational isomerism for EtSiCl<sub>3</sub> (I), EtSiHCl<sub>2</sub> (II), and EtSiH<sub>2</sub>Cl (III). The total frequencies and normal coordinates were calculated for all theoretically possible equilibrium configurations of I, and for the gauche and trans rotamers of II and III. The Mayants method of calcns. was used (CA 63: 13024f). The comparison of exptl. and calculated results shows that, in the crystalline state of II, the trans equilibrium configuration is preserved, whereas III, under very slow crystallization, retains the gauche equilibrium configuration. In liquid and vapor state, the gauche-trans or the trans-gauche forms of II and III mols. are present in dynamic equilibrium. Values for the energy difference between the gauche and trans isomers in the liquid phase were: II, 0.4 kcal./mole; III, -0.3 kcal./mole. The concentration ratio of the isomers was determined at 250°K., molar fractions of the gauche forms of II and III being 0.47 and 0.78, resp. The potential barriers of internal rotation for I, II, and III were calculated by the Magnasco method (CA 60: 7481c).

L3 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1960:9969 CAPLUS  
DOCUMENT NUMBER: 54:9969

ORIGINAL REFERENCE NO.: 54:2008h-i

TITLE: Molecular structures of cyclohexene derivatives. V. Mutually convertible isomers of 4-bromo-1-cyclohexene

AUTHOR(S): Sakashita, Kiyoshi

CORPORATE SOURCE: Hitachi Research Lab.

SOURCE: Nippon Kagaku Zasshi (1959), 80, 972-6

CODEN: NPKZAZ; ISSN: 0369-5387

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 53. 6762h. The Raman and infrared spectra of 4-bromo-cyclohexene were recorded. Two mutually convertible isomers, i.e., inversion isomers, coexist in the liquid as well as in the gaseous state. The energy difference between these 2 isomers in the liquid is about 50 cal./mole, the a-form (axial) being more stable than the e-form (equatorial). The abundance ratio of the 2 isomers in the vapor state is nearly equal to that in the liquid state.

L3 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1957:43156 CAPLUS

DOCUMENT NUMBER: 51:43156

ORIGINAL REFERENCE NO.: 51:8019c-d

TITLE: Isomerization of isopropenylcyclobutane on silica gel under conditions of adsorptional chromatographic analysis

AUTHOR(S): Kazanskii, B. A.; Lukina, M. Yu.; Nakhapetyan, L. A.; Aleksanyan, V. T.; Sterin, Kh. E.

CORPORATE SOURCE: N. D. Zelinskii Inst. Org. Chem., Moscow

SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1956) 1421-2

CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. Arbuzon and Isaera, C.A. 49, 1654i. Examination of the products obtained after room temperature chromatographic adsorption of isopropenylcyclobutane on SiO<sub>2</sub> gel, showed by Raman spectra, that the substance isomerizes to mixed 1,2- and 1,1-dimethylcyclopentanes, the former in 70/15 ratio of trans-cis isomers.

L3 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1954:48782 CAPLUS

DOCUMENT NUMBER: 48:48782

ORIGINAL REFERENCE NO.: 48:8630e-g

TITLE: The solvent effect on the abundance ratios of isomers of trans-1,4-dihalocyclohexanes

AUTHOR(S): Yoshino, Tsuneo

CORPORATE SOURCE: Tokyo Inst. Technol.

SOURCE: Nippon Kagaku Kaishi (1921-47) (1954), Pure Chem. Sect. 75, 592-5

CODEN: NIKWAB; ISSN: 0369-4208

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB There are 2 inversion isomers of trans-1,4-dihalocyclohexane, i.e. p,p-type and e,e-type, where p and e stand for perpendicular and equatorial, resp. Both of them, have the symmetry of C<sub>2h</sub> and are nonpolar. The mol. model of each of the 2 isomers reveals that its form can well be approximated by a prolate ellipsoid of rotation and that the positions of two C-Cl bond moments lie on the principal axis of rotation of the ellipsoid. The reaction field acting on a mol. was calculated from the assumed geometry of the mol. From the stabilizing effect due to this field, which depends on the dielec. constant of the surrounding medium, the dependence of the abundance ratio of isomers on solvents was derived. It was compared with the ratio obtained from the intensities of infrared absorptions or of Raman lines of these isomers in various solvents. The agreement was good.

L3 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1954:5958 CAPLUS

DOCUMENT NUMBER: 48:5958

ORIGINAL REFERENCE NO.: 48:1087d-h

TITLE: Molecular structure of cyclohexene derivatives. I. Molecular structure of 4,5-dichloro-1-cyclohexene

AUTHOR(S): Sakashita, Kiyoshi

CORPORATE SOURCE: Tokyo Inst. Technol.

SOURCE: Nippon Kagaku Kaishi (1921-47) (1953), Pure Chem. Sect. 74, 315-18

CODEN: NIKWAB; ISSN: 0369-4208

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB 4,5-Dichloro-1-cyclohexene was synthesized and its Raman spectrum and dipole moment were measured. The number of the Raman lines in the solid is nearly half that in the liquid at 50°. The mols. in the liquid state are supposed to be of 2 different forms characterized by the Raman lines 690 cm.<sup>-1</sup> and 716 cm.<sup>-1</sup>, resp., whereas in the solid state the mols. of the form characterized by the former frequency disappear. The wave number and the intensity of Raman lines are nearly equal in the pure liquid to those in various solvents. Hence the structure and the abundance ratio of the isomers are not affected by solvents. The dipole moment increases with rising temperature and depends on the kind of solvents. It can be concluded that an isomer with higher moment is less stable than one with smaller moment. Two forms of cyclohexene ring are conceivable, the chair form with C<sub>2</sub> and the boat form with C<sub>3</sub> symmetry. From steric considerations the boat form was ruled out. The chair form of 4,5-dichloro-1-cyclohexene has two possible geometrical isomers, i.e., trans and cis with respect to Cl atoms. Each of them in turn has two inversion isomers, i.e., trans 4p, 5p, trans 4e, 5e, cis 4p, 5e, and cis 4e, 5p, where p and e stand for perpendicular and equatorial, resp. The two cis inversion isomers are antipodes with each other and hence should have the same Raman spectra and the same value for the moment. Therefore, the observed change of moment cannot be explained by the equilibrium between 2 cis isomers. Hence the less stable form was attributed to trans 4e, 5e with (theoretically calculated) higher moment, but the more stable one to trans 4p, 5p. The latter form alone exists in solid state.

L3 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1950:4819 CAPLUS

DOCUMENT NUMBER: 44:4819

ORIGINAL REFERENCE NO.: 44:935g-i

TITLE: Equilibrium ratio of rotational isomers of n-pentane with special reference to its difference from that of 1,2-dichloroethane

AUTHOR(S): Mizushima, Sanichiro; Okazaki, Hiroatsu

SOURCE: Journal of the American Chemical Society (1949), 71, 3411-12

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB For n-C<sub>5</sub>H<sub>12</sub> there can be considered 3 rotational isomers of skeleton; the first one corresponding to the planar, zigzag form (4 consecutive C atoms forming the trans configuration), the second one containing one gauche structure, and the third one containing 2 gauche structures. Of these three forms the first one is the most stable and the third one the most unstable, since in the first form all the movable groups (i.e., CH<sub>3</sub>- or CH<sub>2</sub>-groups) are at the farthest distance apart. The relative intensity of the Raman lines of n-C<sub>5</sub>H<sub>12</sub> was measured at 32° and at -72° and from this exptl. result the energy difference between the rotational isomers was calculated as 0.5 kcal./mol.

L3 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1948:34105 CAPLUS

DOCUMENT NUMBER: 42:34105

ORIGINAL REFERENCE NO.: 42:7235b-f

TITLE: Investigation of the rotation isomerism of 1,2-dihaloethanes by the method of Raman spectra

AUTHOR(S): Aronov, O. L.; Tatevskii, V. M.; Frost, A. V.

CORPORATE SOURCE: Moscow State Univ.

SOURCE: Doklady Akademii Nauk SSSR (1948), 60, 387-90

CODEN: DANKAS; ISSN: 0002-3264

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The equilibrium constant between the 2 forms of 1,2-C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub> was determined from the ratio of the intensities I of 2 Raman lines, by  $K = A(I_2/I_1) = AK'$ , the subscripts 1 and 2 referring, resp., to the frequencies 753 and 653 cm.<sup>-1</sup>, the 1st belonging to the isomer persisting on freezing, the 2nd to that disappearing on freezing (gauche according to Mitsujima); between -31 and +95° (the variation of A in that temperature interval being only about 0.2%, and disregarded),  $K' = \text{constant} = 1.12 \pm 0.09$ , i.e., the ratio of the isomers does not vary in this range. Thus, disappearance of the 2nd isomer can occur only in the solid state or else very close to freezing. In the case of 1,2-C<sub>2</sub>H<sub>4</sub>ClBr, the ratio of the intensities of the 725 and 567 cm.<sup>-1</sup> lines (the former pertaining to the trans form) remains constant =  $1.68 \pm 0.09$  between -13.5 and +93°, and so does the ratio  $725/629 = 2.31 \pm 0.14$ ; only the ratio 725/666 increases slowly with the temperature, from 1.83 to 2.29 between the temperature limits stated. For 1,2-C<sub>2</sub>H<sub>4</sub>Br<sub>2</sub>, the ratios of the intensities 659/551, at 10, 60, 97, and 128°, are 9.61, 4.43, 3.79, and 3.10. Values of the heat Q of transition between the isomers vary in some cases with the Raman lines

used: 1,2-C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub> (from 753/653)  $0 \pm 140$  cal./mole; 1,2-C<sub>2</sub>H<sub>4</sub>ClBr (725/567)  $0 \pm 176$ , (725/629)  $0 \pm 176$ , (725/666)  $395 \pm 160$ ; 1,2-C<sub>2</sub>H<sub>4</sub>Br<sub>2</sub> (659/551)  $-2160 \pm 180$  (between 10 and 128°), (659/551)  $-2220 \pm 230$  (between 10 and 97°), (659/551)  $-2890 \pm 360$  (between 10 and 60°), average  $-2420 \pm 250$ .

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ACCESSION NUMBER: 1947:30801 CAPLUS

DOCUMENT NUMBER: 41:30801

ORIGINAL REFERENCE NO.: 41:6154g-i

TITLE: Raman effect and dipole moment in relation to free rotation. XVI. Dielectric constant of gaseous 1,2-dichloroethane and the equilibrium ratio of rotational isomers

AUTHOR(S): Watanabe, Itaru; Midzushima, San-ichiro; Morino, Yonezo

SOURCE: Scientific Papers of the Institute of Physical and Chemical Research (Japan) (1942), 39, 401-9

CODEN: SPIPAG; ISSN: 0020-3092

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Dielec. consts. of gaseous ClH<sub>2</sub>CCH<sub>2</sub>Cl were measured at different temps. under various pressures. From these results together with the results of the Raman spectra, the partition functions of the trans and gauche mols. were calculated. The equilibrium ratio and the energy difference between the isomers were subsequently obtained. From the intensity ratio of Raman lines observed in the gaseous and the liquid state, the equilibrium ratio in the liquid state also was determined. The gauche mols. are more abundant than the trans molecules in the liquid state; the opposite is true in the gaseous state. By means of Onsager's formula on the dipole moment in the liquid state, the equilibrium ratio obtained was checked theoretically.